

New study of shot noise with the nonequilibrium Kubo formula in mesoscopic systems, application to the Kondo effect at a quantum dot

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Recently we have developed a theory of Keldysh formalism for mesoscopic systems. The resulting nonequilibrium Kubo formula for differential conductance makes it possible to propose the new formula of shot noise S_h , and thus to study shot noise in correlated systems at any temperature and any bias voltage. Employing this new approach, we analyze shot noise in the Kondo regime through a quantum dot for the symmetric case at zero temperature. Using the renormalized perturbation theory, we prove that in the leading order of bias voltage S_h equal to noise power at zero temperature conventionally used as shot noise. With S_h , we calculate the Fano factor for a backscattering current I_b : $F_b = S_h/2eI_b$. It is shown that the Fano factor takes the universal form of $F_b = 1 + 4(R-1)^2/(1+5(R-1)^2)$ determined by the Wilson ratio R for arbitrary strength of the Coulomb interaction. Using the Wilson ratio $R = 2$, our result coincides with the fractional value of $F_b = 5/3$ already derived in the Kondo regime.

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1. INTRODUCTION

Mesoscopic devices have made it possible to investigate many-body effect in transport phenomena. A bias voltage applied to a conductor drives the system into a nonequilibrium steady state. These systems thus offer promising opportunities to study the correlated transport out of equilibrium.

Shot noise has been introduced to explore nonequilibrium nature in these systems^{1,2,3}. Originally shot noise was given by the zero temperature value of noise power S defined by the current-current correlation function. It is well known that, if uncorrelated particles with charge q rarely transmit through a conductor, shot noise is given by the Poisson value $S = 2qI$ where I is the current. Therefore in this case, the quantity $S/2I$ has a possibility to determine the unit of charge carriers q , extracted from not only the current^{1,2,3}. In literature, this result is specific to a low transparent conductor without correlation effects. However, the possibility of shot noise has stimulated recent studies in other systems, for instance, correlated systems. There, the ratio $S/2I$ has been estimated as an indication of effective "charge". As a successful example to give a true quasiparticle charge, the fractional charge $e^* = e/3$ in the fractional quantum Hall regime was determined through $S/2I$ ^{4,5}.

Shot noise defined by the noise power has been useful to reveal attractive features at low temperatures. Extension of the concept of the shot noise at finite temperatures may open new possibilities out, however, how do we define shot noise at finite temperatures?

To illustrate the problem we take a quantum dot system as a stringent example⁶. In the noninteracting case, noise power splits into thermal noise $S_t(T^0)$ and shot noise $S_s(T^0)$ as $S^0 = S_t(T^0) + S_s(T^0)$ at any temperature^{1,2,3}, where T^0 is the bare transmission probability. The fact enables us to define the shot noise

as $S^0 - S_t(T^0)$ at any temperature and any bias voltage. With correlation effects, noise power is obtained as $S = S_t(T) + S_s(T) + \Delta S$. If the effect of Coulomb interaction may be included by simply changing T^0 to the full transmission probability T , noise power would be expressed as $S_t(T) + S_s(T)$. Shot noise thus could be defined in the same way as the uncorrelated system. However, an additional term of ΔS contributes to S . From the expression of ΔS , it is not possible to split it into the thermal-noise part and the shot-noise part. Thus in a quantum dot system it has not been possible to extract shot noise from the noise power. Until this point, we have stated the problem for a quantum dot system. However, the problem to define shot noise in correlated systems is a general one, not limited to the quantum dot system.

Recently we have succeeded in extending a theory of Keldysh formalism for mesoscopic systems, and thus provided a basis for the definition of shot noise at any temperature.

In this study, we have focused on a group of mesoscopic systems, typically designed as a correlated conductor attached to extended reservoirs through tunnel barriers. We have specifically examined the density matrix of the Keldysh formalism^{7,8,9} for these systems^{10,11,12}. An attempt to obtain an explicit expression of the density matrix had been already made in Refs.13,14. However, this attempt was not fully successful, since the density matrix still contained infinite series of operators which arose from the formal expansion of the s-matrix. Summing up them, we have thus proven that the density matrix has a form proposed by MacLennan and Zubarev^{15,16,17}. This type of density matrix was also derived by using a C^* algebra^{18,19}.

The resulting density matrix allows us to derive a general expression of differential conductance: $G = \beta S/4 - \beta S_h/4$, where S is the current-current correlation function, and S_h is the non-trivial current-charge correlation

function and $\beta = 1/k_B T$ ¹⁷. We will call it the *nonequilibrium Kubo formula*. Furthermore, the density matrix has made it possible to prove that a steady state is realized, and describe the issue of irreversible processes in Keldysh formalism. Therefore our theory gives a unified description of desirable features in mesoscopic systems out of equilibrium.

Moreover, the nonequilibrium Kubo formula allows us to introduce a natural definition of the shot noise in correlated systems. In fact the current-current correlation function S is noise power, and of course G is differential conductance. With these observable quantities, the nonequilibrium Kubo formula is written into $S_h = S - 4k_B T G$, and thus we propose the current-charge correlation function S_h as the new definition of the shot noise. This concept has been confirmed in a noninteracting quantum dot by explicitly calculating S , G and the new formula S_h with the Keldysh Green function. The resulting relation among physical quantities is called as the *nonequilibrium identity*. Thus we can compare theoretically calculated S_h at a certain temperature with $S - 4k_B T G$ determined from S and G measured in experiments. Therefore, the nonequilibrium Kubo formula makes it possible to give a new perspective on studies of shot noise at any temperature in correlated systems.¹⁷

Our aim in this paper is to apply this new approach to the quantum dot system in the Kondo regime by analyzing shot noise at low bias voltages.

First, we briefly sketch recent studies of shot noise in the Kondo regime. In these studies shot noise is defined by the noise power S at zero temperature. Theoretically shot noise was investigated in the s-d limit²⁰. When a bias voltage eV is larger than the Kondo temperature T_K , with decreasing the bias voltage shot noise increases logarithmically as is well known in the Kondo systems. Close to the unitarity limit of $eV < T_K$, shot noise is suppressed as

$$S = \frac{2e^2}{h} |V| \frac{\Gamma_L - \Gamma_R}{\Gamma_L + \Gamma_R} + \frac{4e^3}{h} \frac{\gamma}{3} |V| \left(\frac{eV}{T_K} \right)^2 + \dots, \quad (1)$$

where $\Gamma_{L,R}$ are the resonance widths between dot and left and right leads. The Fermi-liquid fixed point Hamiltonian H ^{21,22} is used in calculations.

In recent studies^{23,24}, the Fermi-liquid features in eq.(1) have been reexamined at zero temperature. The fixed point Hamiltonian is characterized by a one-particle scattering and a two-particle scattering. They give corrections to the $\pi/2$ phase shift in the unitarity limit: a frequency-linear phase shift and a quasiparticle-distribution-linear phase shift.

As a result, a current $I_b \equiv -e\partial_t(N_{LH}(t) - N_{RH}(t))$ describes a reduction from the perfect transmission for the $\pi/2$ phase shift in the unitarity limit, which is the definition of the backscattering current in Refs.23,24. Here $N_{L,R}$ express particle-number operators in left and right leads and $A_H(t)$ is the Heisenberg representation for an operator A .

At zero temperature, the observable current is defined by $I = 2e^2 V/h - I_b$, where $I_u = 2e^2 V/h$ is the current in the unitarity limit. Since $2e^2 V/h$ becomes a constant value, noise power given by the current-current correlation function is rewritten as

$$S = \int_{-\infty}^{\infty} dt \langle \{ \delta I_{bH}(t), \delta I_{bH}(0) \} \rangle. \quad (2)$$

Therefore the shot noise is determined by only the backscattering current when $eV < T_K$.

On the basis of this fact, using $S/2I_b$, it has been attempted to estimate an effective "charge" for the backscattering current²³. In the present work we will discuss the Fano factor $F_b = S/2eI_b$ in units of charge e

In Ref.23, the symmetric case $\Gamma_L = \Gamma_R$ is especially focused on. This condition makes the leading order of S in the bias voltage $\mathcal{O}(V^3)$ as in eq.(1). Then, the leading order of I_b also becomes $\mathcal{O}(V^3)$. In the symmetric case, $F_b = S/2eI_b$ results in a universal fractional value up to $\mathcal{O}(V^3)$

$$F_b = \frac{S}{2eI_b} = \frac{5}{3}, \quad (3)$$

It has been pointed out that this universal enhancement from the unity originates from the two-particle backscattering.

This universal feature has stimulated further studies: in the context of the full counting statistics²⁵ this result has been reproduced, and a shot-noise measurement has been reported on $F_b = 5/3$ close to the unitarity limit at low bias voltages²⁶. We address this topic from our point of view.

In this paper, we begin with a brief review of the generalization of the Kubo formula into a nonequilibrium situation and shot noise in Sec.2. In Sec.3 applying our new concept to a quantum dot system described by the Anderson model, we investigate the shot noise and the Fano factor in the Kondo regime. We concentrate on the symmetric case at zero temperature. At zero temperature the nonequilibrium Kubo formula yields $S = S_h$. Thus, using the renormalized perturbation theory, we calculate noise power S and shot noise S_h independently up to the leading order for the symmetric case: $\mathcal{O}(V^3)$ and show that they are identical. The backscattering current is also calculated up to $\mathcal{O}(V^3)$. Finally we will discuss the universal feature of the Fano factor for any Coulomb interaction up to $\mathcal{O}(V^3)$.

2. SHOT NOISE AND NONEQUILIBRIUM KUBO FORMULA

We start with a brief summary of shot noise and the nonequilibrium Kubo formula based on Keldysh formalism for mesoscopic systems in nonequilibrium steady states¹⁷.

2.1. density matrix

Our starting point is the Hamiltonian for a class of mesoscopic systems: a correlated conductor H_c attached to left and right infinite reservoirs $H_{L,R}$ through boundary couplings $H_{cL,R}$. For instance a quantum dot system is a typical example of them. The Hamiltonian is described as

$$H \equiv H_c + H_L + H_R + H_{cL,R}. \quad (4)$$

H_c is given by noninteracting and interacting terms as $H_c \equiv H_{c0} + H_{c1}$. Each reservoir must be sufficiently large to behave as a good thermal bath.

In a conventional explanation of Keldysh formalism, it seems that concepts such as the Keldysh contour, and the Keldysh Green function are stressed⁷. In contrast, our main argument is to examine the early stage of Keldysh formalism where the perturbation term is adiabatically turned on.

To begin with, we divide H into an unperturbed term $H_0 \equiv H_{c0} + H_L + H_R$ and a perturbation term $H_1 \equiv H_{cL,R} + H_{c1}$ ^{10,11,12}. To adiabatically introduce the perturbation term, we use a time-dependent Hamiltonian as $H_{\epsilon t} \equiv H_0 + e^{-\epsilon|t|}H_1$.

The initial state at $t_0 = -\infty$ is determined by the three separated systems in H_0 : left and right reservoirs and the conductor which have different chemical potentials $\mu_{L,R}$, μ_c . We define a bias voltage as $eV/2 \equiv (\mu_L - \mu_R)/2$ and an averaged chemical potential $\mu \equiv (\mu_L + \mu_R)/2$, where $\mu = \mu_c$ is assumed. The origin of energy is set to $\mu = \mu_c = 0$. As a result the initial density matrix is given by

$$\rho_0 = e^{-\beta(H_0 - eV/2(N_L - N_R) - \Omega_0)}. \quad (5)$$

$[H_0, N_L - N_R] = 0$ is assumed throughout. The initial thermodynamic potential is chosen to satisfy $\text{Tr}\{\rho_0\} = 1$, $\Omega_0 = -1/\beta \ln \text{Tr} e^{-\beta(H_0 - eV/2(N_L - N_R))}$.

The time evolution of the density matrix $\rho_\epsilon(t)$ is determined by the Neumann equation. With $\rho_\epsilon(t)$, the expectation value of any operator \mathcal{O} is defined by $\text{Tr}\{\rho_\epsilon(t)\mathcal{O}\}$. It is transformed as

$$\text{Tr}\{\rho_\epsilon(t)\mathcal{O}\} = \text{Tr}\{\rho_\epsilon(0)\mathcal{O}_H(t)\}, \quad (6)$$

where the Heisenberg representation is given by $\mathcal{O}_H(t) = S_\epsilon(0, t)\mathcal{O}(t)S_\epsilon(t, 0)$ and $\mathcal{O}(t) = e^{iH_0 t}\mathcal{O}e^{-iH_0 t}$.

Here in order to avoid confusion, we comment on the time dependence of the expectation value. It is determined by only the Heisenberg representation of an operator \mathcal{O} as shown in the right-hand side of eq.(6). Concerning the density matrix, it is sufficient to consider $\rho_\epsilon(0)$ at $t = 0$. We thus consider a specific time of $t = 0$, but until this point we do not use any assumption either the steady state is realized at $t = 0$ or not. After taking a limit of $\epsilon \rightarrow 0$, the system reaches a steady state. Later we will return back to this point in Sec.2.4.

We thus focus on the density matrix $\rho_\epsilon(0) \equiv \bar{\rho}_\epsilon$ which is given by a formal solution of the Neumann equation

$$\bar{\rho}_\epsilon = S_\epsilon(0, -\infty)\rho_0 S_\epsilon(-\infty, 0). \quad (7)$$

Using the unitarity of $S_\epsilon(0, -\infty)S_\epsilon(-\infty, 0) = 1$, $\bar{\rho}_\epsilon$ becomes

$$\bar{\rho}_\epsilon = \exp\{-\beta(S_\epsilon(0, -\infty)H_0 S_\epsilon(-\infty, 0) - V S_\epsilon(0, -\infty)e/2(N_L - N_R)S_\epsilon(-\infty, 0) - \Omega_0)\}. \quad (8)$$

To proceed calculations, we have to compute a type of quantity

$$\bar{A}_\epsilon \equiv S_\epsilon(0, -\infty)A S_\epsilon(-\infty, 0). \quad (9)$$

We have two cases in our mind: $A = H_0$ and $A = e/2(N_L - N_R)$, where we suppose that A satisfies $[A, H_0] = 0$. The critical step in calculations is to derive¹⁷

$$\bar{A}_\epsilon = A + \int_{-\infty}^0 dt e^{-\epsilon|t|} J_{AH}(t). \quad (10)$$

The "current" for the operator A is defined as

$$J_{AH}(t) \equiv -\frac{\partial}{\partial t} A_H(t). \quad (11)$$

Technically eq.(10) is sufficient to calculate the density matrix. However, we shortly discuss eq.(10), leading to deeper understanding of the nonequilibrium nature in Keldysh formalism. Integration by parts in eq.(10) yields

$$\bar{A}_\epsilon = \epsilon \int_{-\infty}^0 dt e^{-\epsilon|t|} A_H(t). \quad (12)$$

Thus \bar{A}_ϵ expresses a long-time average of A in the limit $\epsilon \rightarrow 0$. In fact, \bar{A}_ϵ defined by eq.(12) represents nothing but the invariant part of an operator A , introduced by Zubarev¹⁵. We have thus proven that the adiabatic introduction of H_1 in Keldysh formalism corresponds to taking the invariant part by Zubarev. We revisit this concept to discuss steady states and irreversible processes in Sec.2.4.

We use eq.(10) in two cases: $A = H_0$ and $A = e/2(N_L - N_R)$ where the "currents" are defined by energy change $J_{eH}(t)$ and charge current $J_{cH}(t)$ using eq.(11), respectively. Substituting them into eq.(8) yields

$$\bar{\rho}_\epsilon = \exp\left\{-\beta\left(H_0 + \int_{-\infty}^0 dt e^{-\epsilon|t|} J_{eH}(t) - eV/2(N_L - N_R) - V \int_{-\infty}^0 dt e^{-\epsilon|t|} J_{cH}(t) - \Omega_0\right)\right\}. \quad (13)$$

The density matrix of Keldysh formalism thus becomes a type of the nonequilibrium statistical operators initiated by MacLennan and Zubarev^{15,16}. This form was also obtained by the C^* algebra^{18,19}.

2.2. nonequilibrium Kubo formula

The resultant density matrix makes it possible to generalize the Kubo formula for conductance into a nonequilibrium steady state. For convenience, in this work we introduce a bra-ket notation: $\langle O \rangle \equiv \lim_{\epsilon \rightarrow 0} \text{Tr}\{\bar{\rho}_\epsilon O\}$. The current is thus denoted as

$$I \equiv \langle J_H(t) \rangle = \langle J \rangle, \quad (14)$$

where in the last equality of eq.(14), a steady-state feature later proved in Sec.2.4 is used. From the current, differential conductance is given as

$$G \equiv \frac{\partial I}{\partial V}. \quad (15)$$

Eq.(14) shows that the current I depend on a bias voltage V only through the density matrix $\bar{\rho}_\epsilon$. To obtain G , $\partial \bar{\rho}_\epsilon / \partial V$ should be calculated. Thus G is given by

$$G = \lim_{\epsilon \rightarrow 0} \beta \text{Tr} \left\{ J \left(e/2(N_L - N_R) + \int_{-\infty}^0 dt e^{-\epsilon|t|} J_H(t) + \frac{\partial \Omega_0}{\partial V} \right) \bar{\rho}_\epsilon \right\}. \quad (16)$$

Using the initial thermodynamic potential Ω_0 and $S_\epsilon S_\epsilon^\dagger = 1$, $\partial \Omega_0 / \partial V$ is calculated as

$$\lim_{\epsilon \rightarrow 0} \frac{\partial \Omega_0}{\partial V} = -e/2 \langle N_L - N_R \rangle + \int_{-\infty}^0 dt e^{-\epsilon|t|} \langle J_H(t) \rangle.$$

Thus the inside of (...) in eq.(16) is expressed by a fluctuation of an operator: $\delta \bar{A}_\epsilon \equiv \bar{A}_\epsilon - \langle \bar{A}_\epsilon \rangle$. In fact, \bar{A}_ϵ just expresses the invariant part of $A = e/2(N_L - N_R)$ in eq.(10). For simplicity we abbreviate it \bar{A}_ϵ for a while. Furthermore, using $\langle B\delta C \rangle = \langle \delta B\delta C \rangle$ for any operators B and C , eq.(16) is rewritten into $G = \beta \langle \delta J \delta \bar{A}_\epsilon \rangle$.

Here we symmetrize the expression of $G = \beta \langle \delta J \delta \bar{A}_\epsilon \rangle$. The current operator J and \bar{A}_ϵ do not commute, but it is possible to transform to the inverse order of $\langle \delta \bar{A}_\epsilon \delta J \rangle$. Using $S_\epsilon [H_0, e/2(N_L - N_R)] S_\epsilon^\dagger = 0$, \bar{A}_ϵ is proven to commute with $\bar{\rho}_\epsilon$. With a cyclic permutation inside the trace, $G = \beta \langle \delta J \delta \bar{A}_\epsilon \rangle$ can be written into $G = \beta \langle \delta \bar{A}_\epsilon \delta J \rangle$. We have thus obtain two different expression of G .

Moreover each form of G is characterized by the time-integral over negative t . It is rewritten into one over positive t using the steady-state feature which will be discussed in eq.(24). Consequently, four different expressions of G are derived. Symmetrizing them yields

$$G = \frac{\beta}{4} \langle \{ \delta J, e(\delta N_L - \delta N_R) \} \rangle + \frac{\beta}{4} \int_{-\infty}^{\infty} dt \langle \{ \delta J_H(t), \delta J_H(0) \} \rangle, \quad (17)$$

where $\{B, C\} = BC + CB$ represents the anticommutation relation.

We have found that differential conductance G is determined by a current-current correlation function, and an unusual current-charge correlation function. In the linear response regime for G : $V = 0$, we can show that

$$\langle \{ \delta J, e(\delta N_L - \delta N_R) \} \rangle_{V=0} = 0, \quad (18)$$

and thus eq.(17) reduces to the standard Kubo formula. Away from the linear response regime, the current-current correlation function gives a naive extension from the relation between fluctuation and dissipation. On the other hand, the current-charge correlation function gives an intriguing modification far from the linear response regime. In conclusion we have succeeded in obtaining a *nonequilibrium Kubo formula* in mesoscopic systems.

2.3. shot noise

We reexamine the nonequilibrium Kubo formula in view of physical quantities. As measurable quantities, there are differential conductance G and noise power given by the current-current correlation function S

$$S = \int_{-\infty}^{\infty} dt \langle \{ \delta J_H(t), \delta J_H(0) \} \rangle. \quad (19)$$

At a steady state noise power at zero frequency dominates.

On the other hand, we define the current-charge correlation function as S_h

$$S_h = -\langle \{ \delta J, e(\delta N_L - \delta N_R) \} \rangle. \quad (20)$$

The nonequilibrium Kubo formula in eq.(17) leads to the relation among S_h and two observable quantities G and S

$$S_h = S - 4k_B T G. \quad (21)$$

As stated in the introduction, in uncorrelated systems shot noise is given by $S^0 - S_t(T^0)$. Considering the fact that the thermal noise $S_t(T^0) = 4k_B T G^0$, S_h in eq.(21) suggests the natural extension of the shot noise. Therefore, we propose to define the shot noise by the current-charge correlation function S_h at arbitrary temperature and bias voltage in correlated systems.

As a result, eq.(21) expresses the relation among physical quantities out of equilibrium. Thus we will call it a *nonequilibrium identity*. In the linear response regime, as discussed previously the current-charge correlation function vanishes, and thus $S_h = 0$. Eq.(21) then goes back to the Nyquist-Johnson relation $S(0) = 4k_B T G(0)$. On the other hand, at zero temperature eq.(21) shows that S_h indeed equals to S at $T = 0$ which is nothing but the original definition of the shot noise.

2.4. steady state

Having discussed consequence of the density matrix on the transport property: the nonequilibrium Kubo formula and shot noise, here we turn to others: irreversible processes and steady states in Keldysh formalism.

We have shown that eq.(10), more explicitly eq.(12) corresponds to the invariant part of an operator A discussed by Zubarev. Originally, this concept was introduced in a local equilibrium system. Zubarev could show that the entropy production was positive in the linear response regime, and thus concluded that the method could describe dissipations. Following the same analysis, it is possible to prove that Keldysh formalism have the same feature as Zubarev theory.

Secondly we discuss steady states. We have shown in Ref.17 that the commutation relation between the invariant part and the Hamiltonian satisfies

$$\lim_{\epsilon \rightarrow 0} [\bar{A}_\epsilon, H_{\epsilon t}] = \lim_{\epsilon \rightarrow 0} -i\epsilon(\bar{A}_\epsilon - A). \quad (22)$$

Assuming that \bar{A}_ϵ exists in the limit $\epsilon \rightarrow 0$, the r.h.s. of eq.(22) vanishes. In $\epsilon \rightarrow 0$ the invariant part commutes with the Hamiltonian, and thus conserves.

This result is crucial for the proof that a steady state is realized in the limit $\epsilon \rightarrow 0$. Using a similar technique to derive eq.(10), the expectation value of an operator \mathcal{O} is rewritten into

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \text{Tr}\{\bar{\rho}_\epsilon \mathcal{O}_H(t)\} &= \lim_{\epsilon \rightarrow 0} \text{Tr}\{\bar{\rho}_\epsilon \mathcal{O}\} \\ &+ \lim_{\epsilon \rightarrow 0} \int_0^t dt' \text{Tr}\{i[\bar{\rho}_\epsilon, H_{\epsilon t'}] J_{\mathcal{O}H}(t-t')\}. \end{aligned} \quad (23)$$

The definition of $\bar{\rho}_\epsilon$ in eq.(7) shows that the density matrix itself in fact becomes an invariant part. As a consequence the commutation relation $[\bar{\rho}_\epsilon, H_{\epsilon t'}]$ in eq.(23) vanishes in the limit $\epsilon \rightarrow 0$, leading to

$$\lim_{\epsilon \rightarrow 0} \text{Tr}\{\bar{\rho}_\epsilon \mathcal{O}_H(t)\} = \lim_{\epsilon \rightarrow 0} \text{Tr}\{\bar{\rho}_\epsilon \mathcal{O}\}. \quad (24)$$

We have proven that a steady state is realized in the limit $\epsilon \rightarrow 0$. According to the same analysis, $\langle \mathcal{O}_H(t) \mathcal{O}_H(t') \rangle = \langle \mathcal{O}_H(t-t') \mathcal{O}_H(0) \rangle$ can be also derived.

3. SHOT NOISE IN THE KONDO EFFECT AT A QUANTUM DOT

3.1. Quantum dot system and physical quantities

Now let us turn to the discussion on shot noise through a quantum dot in the Kondo regime. We consider the Anderson model with a single-level,

$$\begin{aligned} H &= \sum_{k\alpha\sigma} \varepsilon_{k\alpha} c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma} + \sum_{\sigma} \epsilon_d n_{\sigma} + U n_{\uparrow} n_{\downarrow} \\ &+ \sum_{k\alpha\sigma} \left(V_{k\alpha} c_{k\alpha\sigma}^\dagger d_{\sigma} + \text{h.c.} \right). \end{aligned} \quad (25)$$

d_{σ}^\dagger and $c_{k\alpha\sigma}^\dagger$ ($\alpha = L, R$) create an electron with spin σ at the dot and the left-right lead respectively. The last term describes the tunneling between the dot and the leads, which determines the resonance width $\Gamma(\omega) = (\Gamma_L(\omega) + \Gamma_R(\omega))/2$ with $\Gamma_{L,R}(\omega) = 2\pi \sum_k |V_{kL,R}|^2 \delta(\omega - \varepsilon_{kL,R})$. In the limit of large band width, the resonance width may be assumed to be a constant $\Gamma = (\Gamma_L + \Gamma_R)/2$.

As discussed in the introduction, we focus on the Kondo effect near the unitarity limit at zero temperature, and investigate shot noise up to $\mathcal{O}(V^3)$. To discuss the unitarity limit, it is natural to concentrate on the symmetric case, $\epsilon_d = -U/2$ and $\Gamma_L = \Gamma_R = \Gamma$.

Traditionally noise power S at zero temperature has been defined as shot noise. In contrast we define the shot noise in general by eq.(20). From the nonequilibrium identity eq.(21) based on the nonequilibrium Kubo formula,

$$S_h = S, \quad (26)$$

holds at zero temperature. Our first aim in this paper is to show that $S = S_h$ holds up to $\mathcal{O}(V^3)$ by explicit calculations of the two quantities. Second aim is to calculate the Fano factor^{23,24,25,26},

$$F_b = \frac{S_h}{2eI_b}, \quad (27)$$

where the backscattering current I_b is defined as $I_b = I_u - I$ with the current I and the current in the unitarity limit I_u .

3.2. Renormalized perturbation theory

For explicit calculations we employ the renormalized perturbation theory (RPT). It was introduced by Hewson^{27,28} in equilibrium, and then extended by Oguri to the quantum dot system under a finite bias voltage²⁹. In this section the RPT applied for the Anderson Hamiltonian in eq.(25) is introduced first in equilibrium, and then out of equilibrium.

The perturbation theory in U for the Anderson model is characterized by a set of parameters: the energy level ϵ_d , the resonance width Γ , and a regularized Coulomb interaction $U/\pi\Gamma$. In the RPT these parameters are substituted by renormalized ones, $\epsilon_d, \Gamma, U/\pi\Gamma \rightarrow \bar{\epsilon}_d, \bar{\Gamma}, \bar{U}/\pi\bar{\Gamma}$. Using ward identities, three parameters are proved to be related with the regularized spin susceptibility $\tilde{\chi}_s \equiv [2\pi\Gamma/(g\mu_B)^2]\chi_s$, charge susceptibility $\tilde{\chi}_c \equiv (\pi\Gamma/2)\chi_c$ and specific heat coefficient $\tilde{\gamma} \equiv (3\Gamma/2\pi k_B^2)\gamma$,

$$\begin{aligned} \tilde{\chi}_s &= \bar{\rho}_\sigma(0)(1 + \bar{U}\bar{\rho}(0))\pi\bar{\Gamma}, \\ \tilde{\chi}_c &= \bar{\rho}(0)(1 - \bar{U}\bar{\rho}(0))\pi\bar{\Gamma}, \\ \tilde{\gamma} &= \bar{\rho}(0)\pi\bar{\Gamma}. \end{aligned} \quad (28)$$

The density of states at the Fermi level is given by

$$\bar{\rho}(0) = \frac{1}{\pi\bar{\Gamma}} \frac{1}{(\bar{\epsilon}_d/\bar{\Gamma})^2 + 1}. \quad (29)$$

Eq.(28) leads to the Fermi liquid relation: $\tilde{\chi}_s + \tilde{\chi}_c = 2\tilde{\gamma}$, thus two quantities $\tilde{\chi}_s$ and $\tilde{\chi}_c$ become independent variables. The Wilson ratio defined as $R \equiv \tilde{\chi}_s/\tilde{\gamma}$ is expressed as $R = 2\tilde{\chi}_s/(\tilde{\chi}_s + \tilde{\chi}_c)$. As another relation, we consider the Friedel sum rule

$$\bar{n} = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{\bar{\epsilon}_d}{\bar{\Gamma}} \right). \quad (30)$$

Thus $\tilde{\chi}_s$, $\tilde{\chi}_c$ and \bar{n} determine the three renormalized parameters

$$\begin{aligned} \bar{\epsilon}_d &= -\sin(2\bar{n}\pi)\Gamma/(\tilde{\chi}_s + \tilde{\chi}_c), \\ \bar{\Gamma} &= 2\sin^2(\bar{n}\pi)\Gamma/(\tilde{\chi}_s + \tilde{\chi}_c), \\ \bar{U}/\pi\bar{\Gamma} &= (R-1)/\sin^2(\bar{n}\pi). \end{aligned} \quad (31)$$

From the bare Hamiltonian the renormalized parameters can be calculated using the exact Bethe ansatz results of $\tilde{\chi}_s$, $\tilde{\chi}_c$ and \bar{n} ³⁰. Alternatively these parameters can be also estimated by the numerical renormalization group²⁸.

Here we comment on the behaviors of these parameters in the s-d limit and in the symmetric case.

In the Kondo regime, according to Nozières³³, we define the Kondo temperature as $T_K = (g\mu_B)^2/\pi\chi_s$. The Bethe ansatz result of χ_s allows us to determine the expression of the Kondo temperature³⁴

$$T_K = \frac{4}{\pi} \sqrt{U\Gamma} \exp \left\{ -\frac{\pi|\epsilon_d||\epsilon_d + U|}{2U\Gamma} \right\}. \quad (32)$$

In the Kondo limit, $\bar{n} \rightarrow 1/2$ and $\tilde{\chi}_c \rightarrow 0$, therefore $R = 2$, $\bar{\epsilon}_d = 0$, and $\pi\bar{\Gamma} = \bar{U}$. Moreover $\bar{\Gamma} = 2\Gamma/\tilde{\chi}_s = (g\mu_B)^2/\pi\chi_s$ is derived. Using the definition of the Kondo temperature, $\bar{\Gamma} = T_K$ is obtained.

The symmetric case gives rise to $\bar{n} = 1/2$, thus $\bar{\epsilon}_d = 0$, and

$$\frac{\bar{U}}{\pi\bar{\Gamma}} = R - 1. \quad (33)$$

Consequently physical quantities are expanded in a power series of $R - 1$ for the symmetric case.

As a check on RPT, the second-order correction in \bar{U} to the self-energy has been calculated up to $\mathcal{O}(\omega^2)$ and $\mathcal{O}(T^2)$ for the symmetric case²⁷ as

$$\bar{\Sigma}_d^r(\omega) = -i \frac{1}{2\bar{\Gamma}} \left(\frac{\bar{U}}{\pi\bar{\Gamma}} \right)^2 (\omega^2 + \pi^2 T^2) + \dots \quad (34)$$

This result is in agreement with the one in Ref.31 where all orders in the bare U are calculated at low frequencies and temperatures. Within $\mathcal{O}(\omega^2)$ and $\mathcal{O}(T^2)$, the second-order contribution in the renormalized \bar{U} thus gives the exact expression. RPT enables us to discuss the exact Fermi-liquid features in the low energy region for all parameter regimes of ϵ_d , Γ , and $U/\pi\Gamma$ from the weak correlation regime to the strong correlation regime.

Having discussed RPT in equilibrium, let us turn to extension into under a finite bias voltage²⁹. Using the renormalized parameters, this procedure is done as follows.

First we introduce Green functions based on Keldysh formalism

$$\begin{aligned} \bar{G}_d(\tau - 0) &\equiv -i\langle T_c d_\sigma(\tau) d_\sigma^\dagger(0) \rangle, \\ \bar{G}_{pkd}(\tau - 0) &\equiv -i\langle T_c c_{pk\sigma}(\tau) d_\sigma^\dagger(0) \rangle, \\ \bar{G}_{dpk}(\tau - 0) &\equiv -i\langle T_c d_\sigma(\tau) c_{pk\sigma}^\dagger(0) \rangle, \\ \bar{G}_{pkp'k'}(\tau - 0) &\equiv -i\langle T_c c_{pk\sigma}(\tau) c_{p'k'\sigma}^\dagger(0) \rangle, \end{aligned} \quad (35)$$

where $\tau = t^\pm$ is the time variable. The lower and upper branch along the Keldysh contour are denoted by $-$ and $+$, and thus Keldysh components are defined as $A(t^\alpha - 0^\beta) \equiv A^{\alpha\beta}(t - 0)$ for $\alpha, \beta = -, +$.

The equation of motion enables us to relate these full Green functions with \bar{G}_d

$$\begin{aligned} \bar{G}_d(\omega) &= g_d^0(\omega) + g_d^0(\omega) \bar{\Sigma}(\omega) \bar{G}_d(\omega) \\ \bar{G}_{pkd}(\omega) &= \bar{V}_{pk} g_{pkpk}^0(\omega) \sigma_z \bar{G}_d(\omega) \\ \bar{G}_{dpk}(\omega) &= \bar{G}_d(\omega) \sigma_z \bar{V}_{pk}^* g_{pkpk}^0(\omega) \\ \bar{G}_{pkp'k'}(\omega) &= g_{pkp'k'}^0(\omega) \delta_{pp'} \delta_{kk'} \\ &\quad + \bar{V}_{pk} g_{pkpk}^0(\omega) \sigma_z \bar{G}_d(\omega) \sigma_z \bar{V}_{p'k'}^* g_{p'k'p'k'}^0(\omega). \end{aligned} \quad (36)$$

\bar{G} represents the matrix $(\bar{G})^{\alpha\beta} \equiv \bar{G}^{\alpha\beta}$ and σ_z is the third Pauli matrix in the $\alpha\beta$ space. Here g^0 refers to $U = 0$ and $V_{L,Rk} = 0$.

As the zeroth-order Green functions in \bar{U} , we consider the initial Green functions $\bar{g} \equiv \bar{G}|_{\bar{U}=0}$, renormalized by $\bar{V}_{L,Rk}$. The initial Green functions are obtained as the solution of the Dyson eq. for $\bar{G}_d|_{\bar{U}=0} \equiv \bar{g}_d$ in eq.(36),

$$\begin{aligned} \bar{g}_d^{--}(\omega) &= (1 - f_{\text{eff}}) \bar{g}_d^r(\omega) + f_{\text{eff}} \bar{g}_d^a(\omega) \\ \bar{g}_d^{-+}(\omega) &= -f_{\text{eff}} (\bar{g}_d^r(\omega) - \bar{g}_d^a(\omega)) \\ \bar{g}_d^{+-}(\omega) &= (1 - f_{\text{eff}}) (\bar{g}_d^r(\omega) - \bar{g}_d^a(\omega)) \\ \bar{g}_d^{++}(\omega) &= -(1 - f_{\text{eff}}) \bar{g}_d^a(\omega) - f_{\text{eff}} \bar{g}_d^r(\omega). \end{aligned} \quad (37)$$

$$\bar{g}_\sigma^r(\omega) = 1/(\omega - \bar{\epsilon}_d + i\bar{\Gamma}), \quad \bar{g}_\sigma^a(\omega) = g^r(\omega)_\sigma^*,$$

$$f_{\text{eff}} = \frac{\bar{\Gamma}_L f_L + \bar{\Gamma}_R f_R}{\bar{\Gamma}_L + \bar{\Gamma}_R}, \quad (38)$$

Here the Fermi distribution function $f_{L,R} = 1/(1 + e^{\beta(\omega \mp eV/2)})$ are not renormalized. Substituting $\bar{G}_d|_{U=0} = \bar{g}_d$ into eq.(36), we get the explicit forms of other initial Green functions \bar{g}_{pkd} , \bar{g}_{dpk} and $\bar{g}_{pkp'k'}$. In the perturbation theory in \bar{U} , we use these initial Green functions \bar{g} .

Using the initial Green function \bar{g}_d , the Dyson equation of \bar{G}_d in eq.(36) is rewritten into

$$\bar{G}_d(\omega) = \bar{g}_d(\omega) + \bar{g}_d(\omega) \bar{\Sigma}_d(\omega) \bar{G}_d(\omega). \quad (39)$$

With a unitary transformation, eq.(39) is reduced to the three-components form. One of them becomes the Dyson equation for the retarded component,

$$\bar{G}_d^r(\omega) = \bar{g}_d^r(\omega) + \bar{g}_d^r(\omega) \bar{\Sigma}_d^r(\omega) \bar{G}_d^r(\omega). \quad (40)$$

The current is expressed as the renormalized form,

$$I = \frac{e}{h} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \bar{T}(\omega) (f_L - f_R), \quad (41)$$

where transmission probability $\bar{T}(\omega)$ is defined as

$$\bar{T}(\omega) = \frac{\bar{\Gamma}_L \bar{\Gamma}_R}{\bar{\Gamma}_L + \bar{\Gamma}_R} \bar{\rho}(\omega), \quad \rho(\omega) = -\frac{1}{\pi} \text{Im} \bar{G}_d^r(\omega) \quad (42)$$

Under a finite bias voltage, the second-order calculation in \bar{U} for $\bar{\Sigma}^r$ has been done for the symmetric case²⁹,

$$\bar{\Sigma}_d^r(\omega) = -i \frac{1}{2\bar{\Gamma}} \left(\frac{\bar{U}}{\pi\bar{\Gamma}} \right)^2 (\omega^2 + (eV)^2 + \pi^2 T^2) + \dots \quad (43)$$

Clearly this corresponds to eq.(34) in the equilibrium limit $V = 0$ as expected, and moreover reproduces the complete result if combined with the Ward identity³².

We substitute $\bar{\Sigma}^r(\omega)$ of eq.(43) to the formal solution of G^r in eq.(40), and calculate the transmission probability with eq.(42)

$$\bar{T}(\omega) = 1 - \frac{\omega^2}{\bar{\Gamma}^2} - \frac{1}{2\bar{\Gamma}^2} \left(\frac{\bar{U}}{\pi\bar{\Gamma}} \right)^2 \left\{ \omega^2 + \frac{3}{4}(eV)^2 \right\} + \dots \quad (44)$$

The resulting transmission probability allows us to calculate the current defined in eq.(41). For later use, we show the current at zero temperature

$$I = \frac{2e^2}{h} V \left\{ 1 - \frac{1 + 5(R-1)^2}{12} \left(\frac{eV}{\bar{\Gamma}} \right)^2 \right\} + \dots \quad (45)$$

$$\rightarrow \frac{2e^2}{h} V \left\{ 1 - \frac{1}{2} \left(\frac{eV}{T_K} \right)^2 \right\} + \dots, \quad \text{s-d limit} \quad (46)$$

where $\bar{U}/\pi\bar{\Gamma} = R - 1$ is used in eq.(45). In the Kondo limit, $R = 2$ and $\bar{\Gamma} = T_K$. The s-d limit result given in eq.(46) completely agrees with the ones in Refs.22,23,24, 25 where the fixed point Hamiltonian are used.

Therefore, for the quantum dot system the second-order calculations in \bar{U} to the self-energy can provide the exact result up to $\mathcal{O}(\omega^2)$, $\mathcal{O}(T^2)$ and $\mathcal{O}(V^2)$. This result leads to the correct expression of current up to $\mathcal{O}(V^3)$, where we need not count higher-order corrections in \bar{U} .

3.3. Calculation of S and S_h

In this section, we consider shot noise for the symmetric case at zero temperature up to $\mathcal{O}(V^3)$, by employing the two definitions of the shot noise, noise power S at $T = 0$, and the new formula for shot noise S_h . Within $\mathcal{O}(V^3)$, in the same way as the current, the second-order calculations in \bar{U} are sufficient to give correct results for S and S_h .

Both the noise power S in eq.(19) and the shot noise S_h in eq.(20) are two-particle Green functions. Generally they are expressed by the bubble-type diagrams

(bubble-diagrams) and the vertex-correction-type diagrams (vertex-diagrams). We use subscripts 1 and 2 to denote contributions from the bubble-diagrams and vertex-diagrams. Thus $S = S_1 + S_2$ and $S_h = S_{h1} + S_{h2}$.

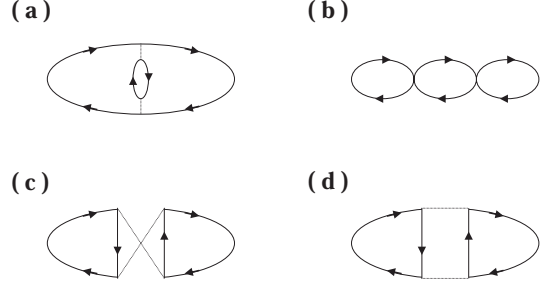


FIG. 1: For the symmetric case, the second-order corrections to the vertex-diagrams.

3.3.1. Noise power S

This section is devoted to the analysis of noise power S . As mentioned previously, RPT in \bar{U} based on Keldysh formalism is employed. We begin with giving a definition of S in the Keldysh form. Considering the steady-state feature in eq.(24), the original S in eq.(19) expressed by the anticommutation relation is rewritten into

$$S = 2 \int_{-\infty}^{\infty} dt \langle T_c J_H(t^+) J_H(0^-) \rangle_L$$

$$= \frac{e^2}{h} \{ 2 \text{Re}(K_a^{+-} - K_b^{+-}) \}. \quad (47)$$

$\langle \dots \rangle_L$ means the linked parts. T_c is the time-ordering operator defined on the Keldysh contour. The time variable t^\pm represent times on the upper and lower branches. It is convenient to classify the current-current correlation functions into $K_{a,b}^{+-}$

$$K_{a,b}^{+-} = \int dt K_{a,b}^{+-}(t-0), \quad (48)$$

where $K_{a,b}^{+-}(t-0) \equiv K_{a,b}(t^+ - 0^-)$. Here

$$K_a(\tau-0) = (i^2/2) \sum_{pp'} \sigma_z^{pp} \sigma_z^{p'p'} \sum_{kk'\sigma\sigma'} \bar{V}_{pk} \bar{V}_{p'k'} \\ \times \langle T_c c_{Hpk\sigma}^\dagger(\tau) d_{H\sigma}(\tau) c_{Hp'k'\sigma'}^\dagger(0) d_{H\sigma'}(0) \rangle_L,$$

$$K_b(\tau-0) = (i^2/2) \sum_{pp'} \sigma_z^{pp} \sigma_z^{p'p'} \sum_{kk'\sigma\sigma'} \bar{V}_{pk} \bar{V}_{p'k'}^* \\ \times \langle T_c c_{Hpk\sigma}^\dagger(\tau) d_{H\sigma}(\tau) d_{H\sigma'}^\dagger(0) c_{Hp'k'\sigma'}(0) \rangle_L$$

$K_{a,b}(\tau-0)$ are also the two-particle Green functions. Thus $K_{a,b}$ is generally given by contributions of the bubble-diagrams $K_{1a,b}$ and the vertex-diagrams $K_{2a,b}$ as

$K_{a,b} = K_{1a,b} + K_{2a,b}$. Applying this relation for S in eq.(47), we define $S_{1,2}$ to satisfy $S = S_1 + S_2$ as follows,

$$\begin{aligned} S_1 &= \frac{e^2}{\hbar} \{2 \operatorname{Re}(K_{1a}^{+-} - K_{1b}^{+-})\} \\ S_2 &= \frac{e^2}{\hbar} \{2 \operatorname{Re}(K_{2a}^{+-} - K_{2b}^{+-})\}. \end{aligned} \quad (49)$$

Thus, explicit calculations of $K_{1,2a,b}$ determine noise power S .

Let us start with the discussion of S_1 . $K_{1a,b}$ are evaluated as

$$\begin{aligned} K_{1a}(\tau - 0) &= (i^2/2) \sum_{pp'} \sigma_z^{pp} \sigma_z^{p'p'} \sum_{kk'\sigma\sigma'} \bar{V}_{pk} \bar{V}_{p'k'} \\ &\quad \times \bar{G}_{dp'k'}(\tau - 0) \bar{G}_{dpk}(0 - \tau) \delta_{\sigma\sigma'}, \\ K_{1b}(\tau - 0) &= (i^2/2) \sum_{pp'} \sigma_z^{pp} \sigma_z^{p'p'} \sum_{kk'\sigma\sigma'} \bar{V}_{pk} \bar{V}_{p'k'}^* \\ &\quad \times \bar{G}_d(\tau - 0) \bar{G}_{p'k'pk}(0 - \tau) \cdot \delta_{\sigma\sigma'} \end{aligned} \quad (50)$$

In the following, we use the Fourier representation.

It is shown that \bar{G}_{dpk} and $\bar{G}_{p'k'pk}$ are related with \bar{G}_d in eq.(36). Technically, these relations are sufficient to proceed further calculations. However, here it is better to comment on a difference between calculations of noise power and shot noise.

Here we concern with the k -sum in eq.(50). In both cases the k -sum is reduced to a form

$$\sum_k \bar{V}_{pk} \bar{G}_{dpk}, \sum_{kk'} \bar{V}_{pk} \bar{V}_{p'k'}^* \bar{G}_{p'k'pk} \rightarrow \sum_k |V_{pk}|^2 g_{pkpk}^0(\omega).$$

$g_{pkpk}^0(\omega)$ are the bare Green functions for the free electrons in leads when $U = 0$ and $V_{pk} = 0$. Thus the analytic properties of $g_{pkpk}^0(\omega)$ are characterized by infinitesimal quantities $\pm i\epsilon$. By performing the k -sum of g_{pkpk}^0 , the δ -function singularities are averaged. Therefore in the full bubble-diagram calculations, the k -sum provides well-defined quantities.

However, in the shot-noise calculations, another type of the k -sum leads to a δ -function singularity. We will discuss this point in the next section.

Let us return back to the main discussion. The relations in eq.(36) allows us to rewrite $2 \operatorname{Re}(K_{1a}^{+-} - K_{1b}^{+-})$ into an expression with \bar{T} ,

$$\begin{aligned} 2 \operatorname{Re}(K_{1a} - K_{1b}) &= \int \frac{d\omega}{2\pi} \{-4\bar{T}^2(\omega)(f_L - f_R)^2 \\ &\quad + 4\bar{T}(\omega)(f_L(1 - f_R) + f_R(1 - f_L))\}. \end{aligned} \quad (51)$$

Using

$$\begin{aligned} f_L(1 - f_R) + f_R(1 - f_L) &= \\ f_L(1 - f_L) + f_R(1 - f_R) + (f_L - f_R)^2, \end{aligned} \quad (52)$$

S_1 can be represented as

$$\begin{aligned} S_1 &= \frac{4e^2}{\hbar} \int d\omega \bar{T}(\omega)(f_L(1 - f_L) + f_R(1 - f_R)) \\ &\quad + \frac{4e^2}{\hbar} \int d\omega \bar{T}(\omega)(1 - \bar{T}(\omega))(f_L - f_R)^2. \end{aligned} \quad (53)$$

We have proven that noise power S_1 for the bubble-diagrams decouples into the thermal-noise part and shot-noise part in the same manner as noninteracting systems^{1,2}. However, in this case the transmission probability is fully renormalized by the Coulomb interaction.

At zero temperature, in S_1 the thermal-noise part vanishes. Consequently we discuss the remaining shot-noise part in the second-line of eq.(53). With \bar{T} given by eq.(44), we evaluate the asymptotic form of S_1

$$S_1 = \frac{4e^3}{\hbar} |V| \left\{ \frac{1}{12} \left(\frac{eV}{\bar{\Gamma}} \right)^2 + \frac{5}{12} (R - 1)^2 \left(\frac{eV}{\bar{\Gamma}} \right)^2 \right\}, \quad (54)$$

where $\bar{U}/\pi\bar{\Gamma} = R - 1$.

Here, let us turn to the discussion of S_2 for the vertex-diagrams. Diagrams up to the second order in \bar{U} are shown in Fig. 1. For the symmetric case, we can show that the contribution from the diagram in (c) cancels out the one from (d), and the one from (b) itself vanishes. We explicitly calculate the remaining diagram in (a).

We calculate K_{2a} up to the second order in \bar{U}

$$K_{2a,b}(\tau - 0) = 2 \int d\tau_1 d\tau_2 F_{a,b}, \quad (55)$$

where

$$\begin{aligned} F_a &= \bar{g}_d(\tau - \tau_1) \sum_{p'} \sigma_z^{p'p'} \sum_{k'} \bar{V}_{p'k'} \bar{g}_{dp'k'}(\tau_1 - 0) \\ &\quad \times \bar{g}_d(0 - \tau_2) \sum_p \sigma_z^{pp} \sum_k \bar{V}_{pk} \bar{g}_{dpk}(\tau_2 - \tau) \\ &\quad \times \bar{U} \bar{g}_d(\tau_1 - \tau_2) \bar{U} \bar{g}_d(\tau_2 - \tau_1), \quad (56) \\ F_b &= \bar{g}_d(\tau - \tau_1) \bar{g}_d(\tau_1 - 0) \times \sum_{pp'} \\ &\quad \sum_{k'} \bar{V}_{p'k'}^* \bar{g}_{p'k'd}(0 - \tau_2) \sigma_z^{p'p} \sum_k \bar{V}_{pk} \bar{g}_{pkd}(\tau_2 - \tau) \\ &\quad \times \bar{U} \bar{g}_d(\tau_1 - \tau_2) \bar{U} \bar{g}_d(\tau_2 - \tau_1). \quad (57) \end{aligned}$$

With eq.(49) S_2 is obtained in the Fourier representation

$$S_2 = \frac{4e^2}{\hbar} c \int d\omega_1 d\omega_2 F_{ab},$$

where $c = \bar{U}^2 \bar{\Gamma}^2 / (2\pi)^2$. F_{ab} is given by

$$\begin{aligned} F_{ab} &= \sum_{\alpha} g_d(\omega_1)^{\alpha-} \sigma_z^{\alpha\bar{\alpha}} g_d(\omega_1)^{+\bar{\alpha}} (f_L - f_R)(\omega_1 + \omega_2) \\ &\quad \times g_d(\omega_2)^{-\alpha} g_d(\omega_2)^{\bar{\alpha}+} (f_L - f_R)(\omega_2) \times \Gamma(\omega_2 - \omega_1), \end{aligned}$$

where $\bar{\alpha} \equiv -\alpha$ and $(f_L - f_R)(\omega) \equiv f_L(\omega) - f_R(\omega)$. The vertex function $\Gamma(\omega)$ is defined as

$$\begin{aligned} \Gamma(\omega) &= \int d\omega' g_d^{-+}(\omega') g_d^{+-}(\omega + \omega') \\ &\simeq \theta(\omega) \frac{2\omega}{\bar{\Gamma}^2} + \theta(\omega - eV) \frac{\omega - eV}{\bar{\Gamma}^2} + \theta(\omega + eV) \frac{\omega + eV}{\bar{\Gamma}^2}. \end{aligned} \quad (58)$$

Performing the frequency-integral gives the explicit form of $\Gamma(\omega)$. In eq.(58) we show the leading-order of $\Gamma(\omega)$.

Finally S_2 becomes

$$S_2 = \frac{4e^2}{h}|V| \left\{ \frac{1}{3}(R-1)^2 \left(\frac{eV}{\Gamma} \right)^2 \right\} + \dots \quad (59)$$

Therefore $S = S_1 + S_2$ is also obtained up to the leading-order in V ,

$$S = \frac{4e^3}{h}|V| \left\{ \frac{1}{12} \left(\frac{eV}{\Gamma} \right)^2 + \frac{5}{12}(R-1)^2 \left(\frac{eV}{\Gamma} \right)^2 + \frac{1}{3}(R-1)^2 \left(\frac{eV}{\Gamma} \right)^2 \right\}. \quad (60)$$

3.3.2. Shot noise S_h

This section is devoted to calculations of the new formula of shot noise

$$S_h = -\langle \{\delta J, e(\delta N_L - \delta N_R)\} \rangle. \quad (61)$$

Originally, S_h contains $4 \times 4 = 16$ two-particle Green functions. The current conservation $\langle J_L + J_R \rangle = 0$ reduces the number to 8 two-particle Green functions. As a preliminary step, we define the reduced S_h in the Keldysh form

$$S_h = \frac{e^2}{h} 2 \operatorname{Re} \{ (K_{LL} + K_{RR}) - (K_{LR} + K_{RL}) \}, \quad (62)$$

where $K_{pp'}$ for $p, p' = L, R$ are given by

$$K_{pp'} = -i \sum_{kk'\sigma\sigma'} V_{pk} \langle T_c c_{Hp\sigma}^\dagger(0^+) d_{H\sigma}(0^+) c_{Hp'k'\sigma'}^\dagger(0^-) c_{Hp'k'\sigma'}(0^-) \rangle_L.$$

The equal-time correlation functions are defined by using the Keldysh branches.

$K_{pp'}$ as the two-particle Green functions are generally given by $K_{1pp'}$ for the bubble-diagrams and $K_{2pp'}$ for the vertex-diagrams. Correspondingly, $S_{h1,2}$ are defined as $S_h = S_{h1} + S_{h2}$:

$$\begin{aligned} S_{h1} &= \frac{e^2}{h} 2 \operatorname{Re} \{ (K_{1LL} + K_{1RR}) - (K_{1LR} + K_{1RL}) \}, \\ S_{h2} &= \frac{e^2}{h} 2 \operatorname{Re} \{ (K_{2LL} + K_{2RR}) - (K_{2LR} + K_{2RL}) \}. \end{aligned} \quad (63)$$

Therefore an evaluation of $K_{1,2pp'}$ determines S_h .

First we discuss $K_{1pp'}$

$$\begin{aligned} K_{1pp'} &= -i \sum_{kk'\sigma\sigma'} \delta_{\sigma\sigma'} \bar{V}_{pk} \bar{G}_{p'k'pk}^{+-}(0) \bar{G}_{dp'k'}^{+-}(0), \\ &= -i \sum_{kk'\sigma\sigma'} \delta_{\sigma\sigma'} \int \frac{d\omega_{12}}{(2\pi)^2} \bar{V}_{pk} \bar{G}_{p'k'pk}^{+-}(\omega_1) \bar{G}_{dp'k'}^{+-}(\omega_2), \end{aligned} \quad (64)$$

where $d\omega_{12} = d\omega_1 d\omega_2$.

Now we examine the k -sum in eq.(64). Applying eq.(36) for the summation over k' , essential part of calculations are reduced to a form

$$\begin{aligned} &\sum_{k'} V_{pk} G_{p'k'pk}^{+-}(\omega_1) G_{dp'k'}^{+-}(\omega_2) \\ &\rightarrow \sum_{k'} |V_{p'k'}|^2 g_{p'k'p'k'}^{0\alpha\beta}(\omega_1) g_{p'k'p'k'}^{0\gamma\delta}(\omega_2). \end{aligned} \quad (65)$$

Notice that the analytic properties of $g_{p'k'p'k'}^{0\alpha\beta}$ are determined by $\pm i\epsilon$ because of the free electrons in leads. Summation of the product of two g^0 with different frequencies ω_1 and ω_2 over k' gives rise to a δ -function singularity when ω_1 is close to ω_2 , and a principal integration. This point is quite different from the one in S_1 .

In contrast, the summation over k in eq.(64) has the same character as the one previously discussed in S_1 . Thus it does not produce the δ -function singularity.

To determine S_{h1} we evaluate $2 \operatorname{Re}(K_{1LL} + K_{1RR})$

$$\begin{aligned} &2 \operatorname{Re}(K_{1LL} + K_{1RR}) = \\ &2 \int \frac{d\omega}{2\pi} \{ \bar{T}(\omega)(1 - \bar{T}(\omega))(f_L - f_R)^2 + a(\omega) - b(\omega) \}. \end{aligned} \quad (66)$$

The term of $\bar{T}(1 - \bar{T})$ and the $a(\omega)$ -term originate from the δ -function term where

$$a(\omega) = \pi^2 \bar{\rho}(\omega)^2 (\bar{\Gamma}_L - \bar{\Gamma}_R) \frac{\bar{\Gamma}_L \bar{\Gamma}_R}{\bar{\Gamma}_L + \bar{\Gamma}_R} (f_L - f_R). \quad (67)$$

The $b(\omega)$ -term originates from the principal integration. We can prove that $b(\omega)$ completely agrees with $a(\omega)$: $b(\omega) = a(\omega)$. As a consequence $2 \operatorname{Re}(K_{1LL} + K_{1RR})$ is characterized by $\bar{T}(1 - \bar{T})$, as expected for shot noise.

Moreover the same type calculations lead to that $2 \operatorname{Re}(K_{1LR} + K_{1RL}) = -2 \operatorname{Re}(K_{1LL} + K_{1RR})$. S_{h1} becomes

$$S_{h1} = \frac{4e^2}{h} \int d\omega \bar{T}(\omega)(1 - \bar{T}(\omega))(f_L - f_R)^2. \quad (68)$$

We conclude that S_{h1} has a shot-noise form, but characterized by the full \bar{T} . Employing eq.(44), the leading-order of S_{h1} can be calculated at zero temperature as

$$S_{h1} = \frac{4e^3}{h}|V| \left\{ \frac{1}{12} \left(\frac{eV}{\Gamma} \right)^2 + \frac{5}{12}(R-1)^2 \left(\frac{eV}{\Gamma} \right)^2 \right\} \quad (69)$$

where $\bar{U}/\pi\bar{\Gamma} = R - 1$.

Having addressed S_{h1} for the bubble-diagrams, let us turn to S_{h2} for the vertex-diagrams. We can confirm that for S_{h2} only the term (a) in Fig.1 remains in the same way as S_2 . Considering this point, the second-order correction to $K_{2pp'}$ are evaluated. The obtained $K_{2pp'}$ for $p, p' = L, R$ decide S_{h2} as follows,

$$S_{h2} = \frac{e^2}{h} \int d\tau_1 d\tau_2 \operatorname{Re} F_h. \quad (70)$$

F_h is given by

$$F_h = -i4 \sum_{p'} \sigma_z^{p'p'} \left[\sum_{k'} \bar{g}_{dp'k'}(\tau_1 - 0^-) \bar{g}_{p'k'd}(0^- - \tau_2) \right] \\ \times \bar{g}_d(0^+ - \tau_1) \sum_p \sigma_z^{pp} \sum_k \bar{V}_{pk} \bar{g}_{dpk}(\tau_2 - 0^+) \\ \times \bar{U} \bar{g}_d(\tau_1 - \tau_2) \bar{U} \bar{g}_d(\tau_2 - \tau_1). \quad (71)$$

Following the discussion of the k -sum in S_{h1} , we find that $[\sum_{k'} \dots]$ in eq.(71) gives the δ -function part and the principal-integration part.

Taking this point into account, we perform calculations of all Keldysh components of $F_h^{\alpha\beta}$, defined by $\tau_1 = t_1^\alpha$ and $\tau_2 = t_2^\beta$ in eq.(71). We discuss relevant $\sum_{\alpha\beta} \text{Re} F_h^{\alpha\beta}$ for S_{h2} . We find that the principal-integration parts in $\sum_{\alpha\beta} \text{Re} F_h^{\alpha\beta}$ vanish. Concerning the δ -function part, $\text{Re} F_h^{--}$, $\text{Re} F_h^{+-}$ and $\text{Re} F_h^{++}$ do not contribute to the leading-order of S_{h2} in V . $\text{Re} F_h^{-+}$ determines the leading-order of S_{h2}

$$S_{h2} = -\frac{4e^2}{\hbar} c' \int d\omega_1 d\omega_2 (f_L(\omega_1 + \omega_2) - f_R(\omega_1 + \omega_2)) \\ \times \bar{g}_d^{+-}(\omega_1) (f_L(\omega_1) - f_R(\omega_1)) \bar{g}^r(\omega_1) \times \Gamma(\omega_2), \quad (72)$$

where $c' = \pi \bar{\Gamma}^2 \bar{U}^2 / (2\pi)^4$. $\Gamma(\omega)$ is the vertex function defined in eq.(58). Employing the asymptotic form of $\Gamma(\omega)$, S_{h2} is evaluated as

$$S_{h2} = \frac{4e^3}{\hbar} |V| \left\{ \frac{1}{3} (R-1)^2 \left(\frac{e\bar{V}}{\bar{\Gamma}} \right)^2 \right\} + \dots, \quad (73)$$

where $\bar{U}/\pi\bar{\Gamma} = R-1$.

Therefore, the asymptotic form of $S_h = S_{h1} + S_{h2}$ is determined as

$$S_h = \frac{4e^3}{\hbar} |V| \left\{ \frac{1}{12} \left(\frac{eV}{\bar{\Gamma}} \right)^2 + \frac{5}{12} (R-1)^2 \left(\frac{eV}{\bar{\Gamma}} \right)^2 \right. \\ \left. + \frac{1}{3} (R-1)^2 \left(\frac{eV}{\bar{\Gamma}} \right)^2 \right\}. \quad (74)$$

Finally we summarize the results of the noise power $S = S_1 + S_2$ and the shot noise $S_h = S_{h1} + S_{h2}$. Subscripts of 1 and 2 represent the contributions from the bubble-diagrams and the vertex-diagrams.

As a check we begin with $S = S_1 + S_2$. Taking the s-d limit leads to $\Gamma \rightarrow T_K$ and the Wilson ratio $R \rightarrow 2$. We find that the resulting asymptotic form of $S = S_1 + S_2$ precisely agrees with the ones obtained as shot noise by using the fixed-point Hamiltonian^{23,24,25}. Up to $\mathcal{O}(V^3)$, the second-order RPT indeed gives the correct result.

We turn to S_h proposed as the new formula of shot noise. Up to the leading order in V , $S_1 = S_{1h}$ and $S_2 = S_{2h}$ are clearly satisfied. Therefore for the symmetric case at zero temperature, S_h precisely agrees with S up to $\mathcal{O}(V^3)$.

3.4. Fano factor F_b

In this section, we would like to argue the Fano factor

$$F_b = \frac{S_h}{2eI_b}. \quad (75)$$

Conventionally, noise power S at zero temperature is treated as shot noise. However, we have proposed S_h as shot noise at any temperature based on the nonequilibrium Kubo formula. Therefore, it is natural to define the Fano factor with S_h in eq.(75). Here I_b expresses the backscattering current^{23,24,25,26}

$$I_b = \frac{2e^2}{\hbar} V - I. \quad (76)$$

The I in eq.(45) gives an expression of $2eI_b$

$$2eI_b = \frac{4e^3}{\hbar} V \left\{ \frac{1}{12} \left(\frac{eV}{\bar{\Gamma}} \right)^2 + \frac{5}{12} (R-1)^2 \left(\frac{eV}{\bar{\Gamma}} \right)^2 \right\}. \quad (77)$$

The backscattering current $2eI_b$ just corresponds to S_{h1} for the bubble-diagrams in eq.(69): $2eI_b = S_{h1}$ for $V > 0$. Consequently $F_b = (S_{h1} + S_{h2})/2eI_b = 1 + S_{h2}/2eI_b$. Using expressions of S_{h2} for the vertex diagrams in eq.(73) and $2eI_b$ in eq.(77), we obtain F_b

$$F_b = 1 + \frac{4(R-1)^2}{1 + 5(R-1)^2}. \quad (78)$$

The first term in F_b originates from S_{h1} . S_{h1} is characterized by only \bar{T} . If correlation effect gives only a change from the bare T^0 to the full \bar{T} , $F_b = 1$ would hold within $\mathcal{O}(V^3)$. Actually, S_{h2} from the vertex-diagrams contributes to F_b . As a result it gives an enhancement factor of the second term in eq.(78). The vertex-diagram is known to describe a kind of the back-flow effect. The back-flow effect enhances the Fano factor for backscattering current. The form of the enhancement in F_b has a universal feature that only the Wilson ratio determines it for any U .

Here we check the resulting F_b in the limit of $U \rightarrow \infty$ and $U \rightarrow 0$. Applying limiting values of the Wilson ratio R for F_b leads to

$$F_b = \begin{cases} \frac{5}{3} & U \rightarrow \infty \quad R = 2 \\ 1 & U \rightarrow 0 \quad R = 1 \end{cases} \quad (79)$$

F_b indeed reproduces the universal fractional value of $F_b = 5/3$ derived in the s-d limit^{23,24,25}, and a naively expected value $F_b = 1$ for a noninteracting system. Therefore F_b given by eq.(78) is an extension for any U from the already obtained value of $F_b = 5/3$ in the s-d limit.

Before closing discussion, we touch on an application of F_b . By using F_b , we may determine the Wilson ratio directly from experiments as follows,

$$R = 1 + \sqrt{\frac{F_b - 1}{9 - 5F_b}}.$$

4. SUMMARY

The nonequilibrium Kubo formula $S_h = S - 4k_B T G$ allows us to propose S_h as the new definition of shot noise in general. Experimentally measured $S - 4k_B T G$ can be compared with a theoretical prediction of S_h at any temperature. Therefore, the nonequilibrium Kubo formula thus opens a new approach to studies of shot noise in correlated systems at any temperature and any bias voltage.

Then, using this approach shot noise through a quantum dot in the Kondo regime has been investigated. For simplicity, the symmetric case has been discussed at zero temperature. At $T = 0$, the nonequilibrium Kubo formula gives $S_h = S$. We have thus analyzed both S and S_h , up to $\mathcal{O}(V^3)$ which is the leading order in V for the symmetric case. The renormalized perturbation theory (RPT) has enabled us to obtain the exact asymptotic form of S and S_h . Both of S and S_h are expressed by two-particle Green functions. Thus they have two types of contributions from the bubble-diagrams and the vertex-diagrams as $S = S_1 + S_2$ and $S_h = S_{h1} + S_{h2}$. It has been shown $S_1 = S_{h1}$ and $S_2 = S_{h2}$ up to $\mathcal{O}(V^3)$. We have concluded that S_h indeed equals S at $T = 0$

which was conventionally defined as shot noise. Finally we have pointed out that $S_{h2}(= S_2)$ from the vertex-diagrams leads to the universal enhancement factor in the Fano factor: $F_b = 1 + 4(R-1)^2/(1+5(R-1)^2)$. This expression includes the result of $F_b = 5/3$ in the Kondo limit by using the Wilson ratio $R = 2$.

Furthermore, we have found that S_1 splits into the thermal-noise part and the shot-noise part with the full transmission probability T . Here, let us recall the fact of $S = S_t(T) + S_s(T) + \Delta S$. In fact, $S_1 = S_t(T) + S_s(T)$. Thus, ΔS describes nothing but the contribution from the vertex-diagrams: $S_2 = \Delta S$. As discussed previously, concerning ΔS it is not clear whether noise power S at a general temperature is split into the thermal-noise part and the shot-noise part. However, it is impossible to ignore the effect of ΔS , even at zero temperature because $S_{h2} = S_2 = \Delta S$ is always relevant as in the universal enhancement factor in F_b .

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